HPC & AI: Accelerating the Design of a Clean, Highly Efficient Gasoline Compression Ignition Engine

Yuanjiang Pei

Aramco Research Center – Detroit

Aramco Services Company

CAESES Users Meeting

Sep. 19, 2019

Berlin, Germany

where energy is opportunity™

Saudi Aramco is a fully integrated energy and chemicals enterprise

336.2
billion
barrels of oil equivalent

10.2
million bpd
crude with blended condensate produced

8.9
billion scfd
of natural gas processed

70,000
employees

Saudi Aramco Prospectus, April 1, 2019

Our Research Footprint

Our worldwide R&D program is led by established award-winning research centers in Dhahran together with other research and technology centers around the world.

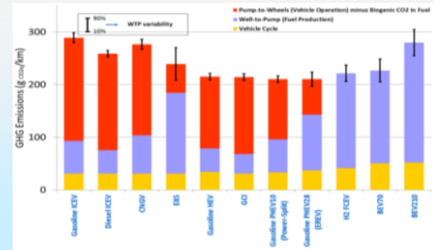
General Use

aramco

Research Focus Areas in Detroit

Strategic Transport Analysis

- Conducts energy and transportation scenario analysis
- Identify the most effective path forward to minimize transportation's carbon footprint.



Passenger Transport Fuels Research

- Innovate fuel and engine t
fuel efficiency (lower CO_2)

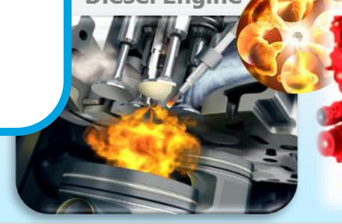
Gasoline Engine

CFD + HPC

Commercial Transport Fuels Research

- Innovate fuel and engine t
emissions and fuel efficiency – Holistic Approach

Diesel Engine



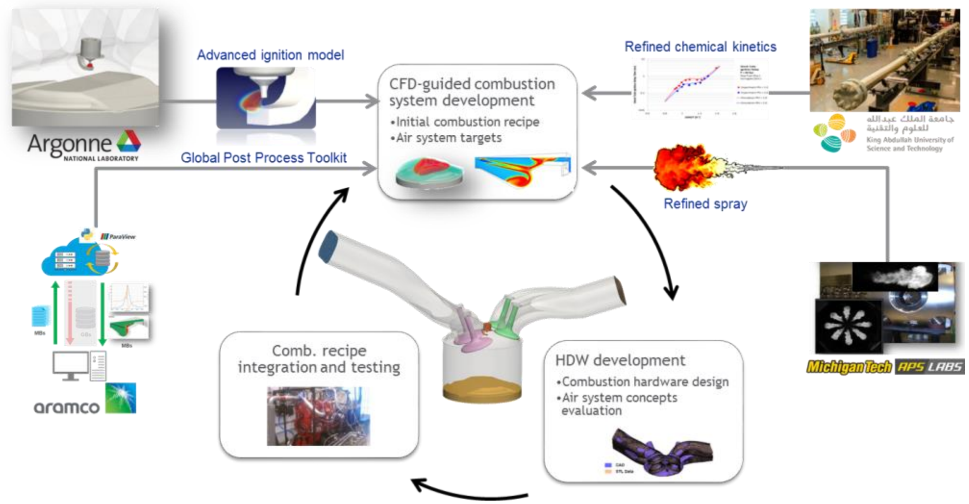
Vehicle Technology Integration

- Combining the pieces together into an integrated vehicle to demonstrate technology viability and performance

General Use

Detroit Research Center Facilities

- Five state-of-the-art fuel and engine performance and emissions transient dynamometers - fully automated
- Four-wheel drive climatic chassis dynamometer
- Aramco engine and vehicle controller - first vehicle operational
- Excellent computational capability



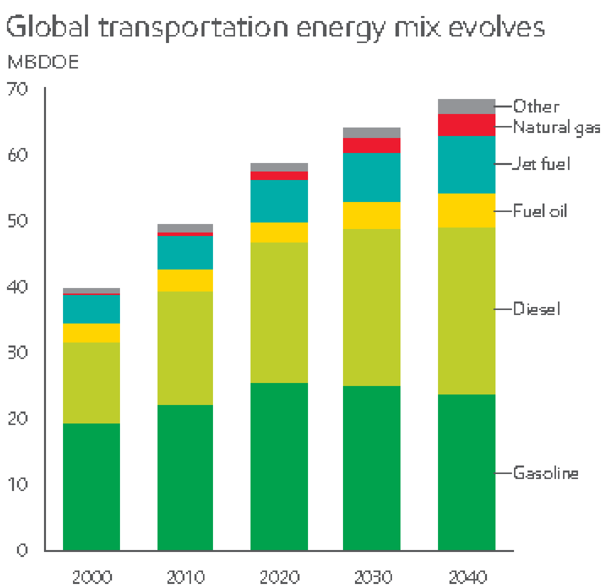
General Use

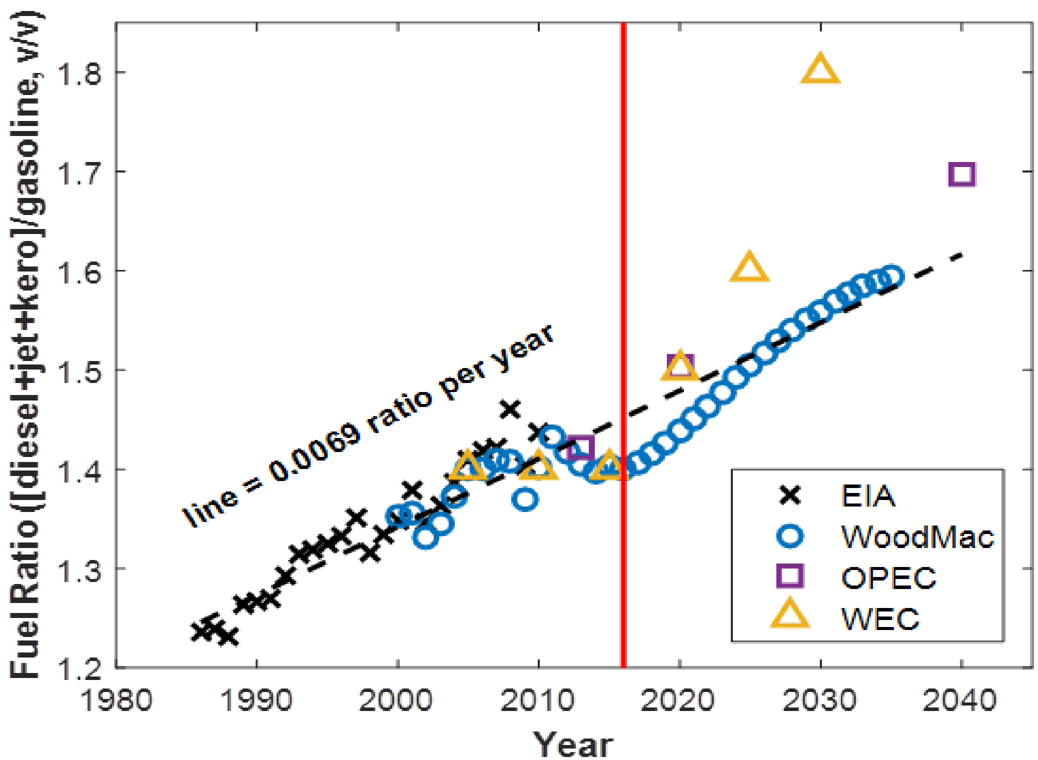
aramco

Commercial Transport Research
Heavy-Duty Gasoline Compression Ignition Engine
-Project Background

Demand Imbalance Scenario

- ➢ Global economic growth drives increase in commercial demand
- ➢ Demand shift likely to produce price imbalance between gasoline and diesel
- ➢ Burning light end fuels efficiently in CI engines becomes economically attractive

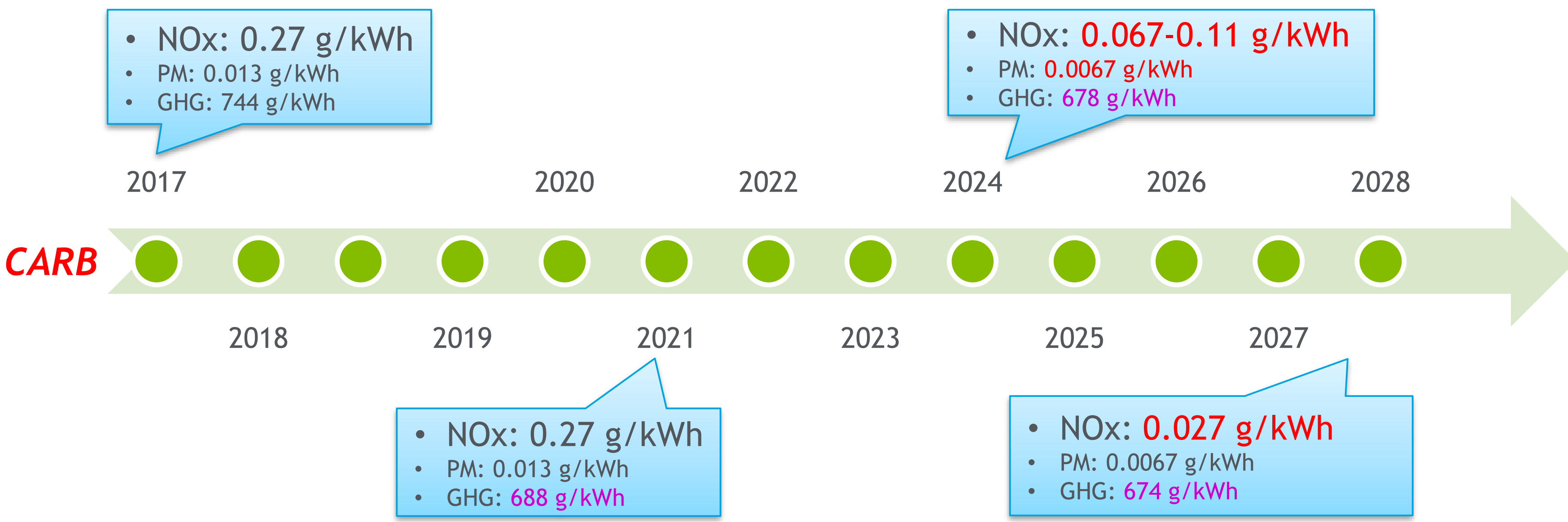




➔ Total cost of ownership pressures will make gasoline range fuels attractive

Regulatory Requirement

- Stringent regulatory demand on reducing criteria pollutants & GHG emissions
- Evolutionary & cost-effective technologies are attractive to manufacturers

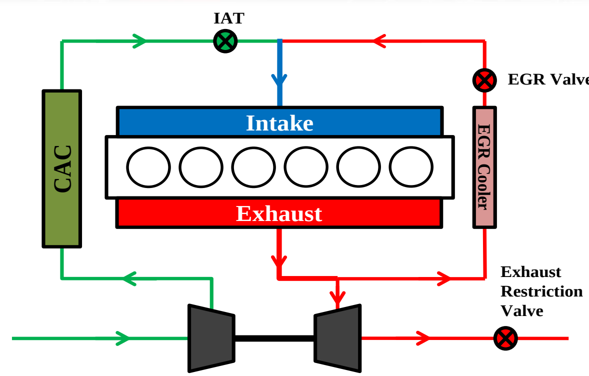


→ **GCI's emissions benefit offers a pathway to meet the regulatory requirements at lower cost**

Test Engine

- Modern heavy duty highway diesel engine that can be installed in all major truck brands – non-road variant also available

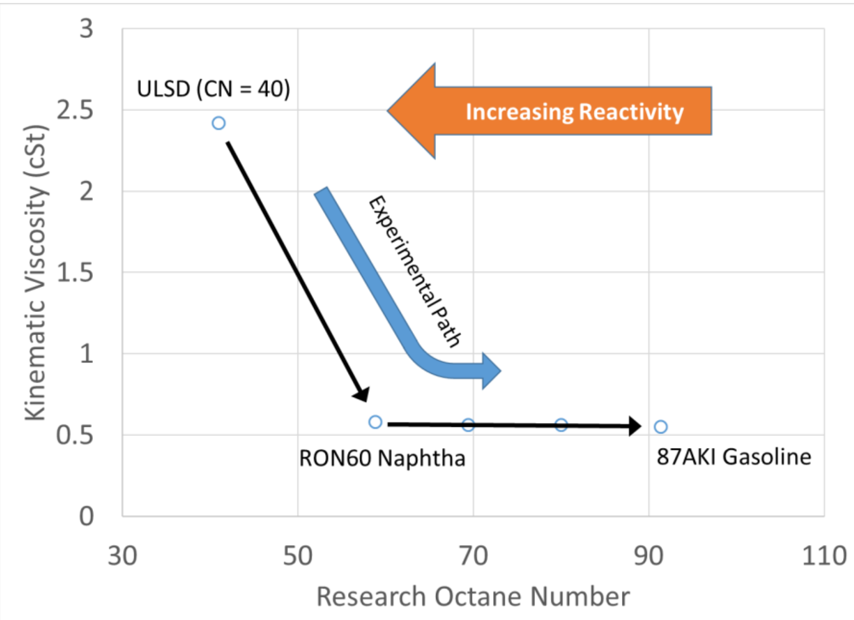
Displacement Volume	14.9 L
Number of Cylinders	6
Bore	137 mm
Stroke	169 mm
Compression Ratio	18.9, variants at 17.3 & 15.7
Diesel Fuel System	2500 bar common-rail
Air System	single-stage VGT high pressure cooled EGR loop charge air cooler
Engine Ratings	450 hp @ 1800 rpm 1750 lb-ft @ 1000 rpm



➔ Aramco purchased a 2013MY Cummins ISX 15L 450hp engine as a research test bed

Fuel Characteristics

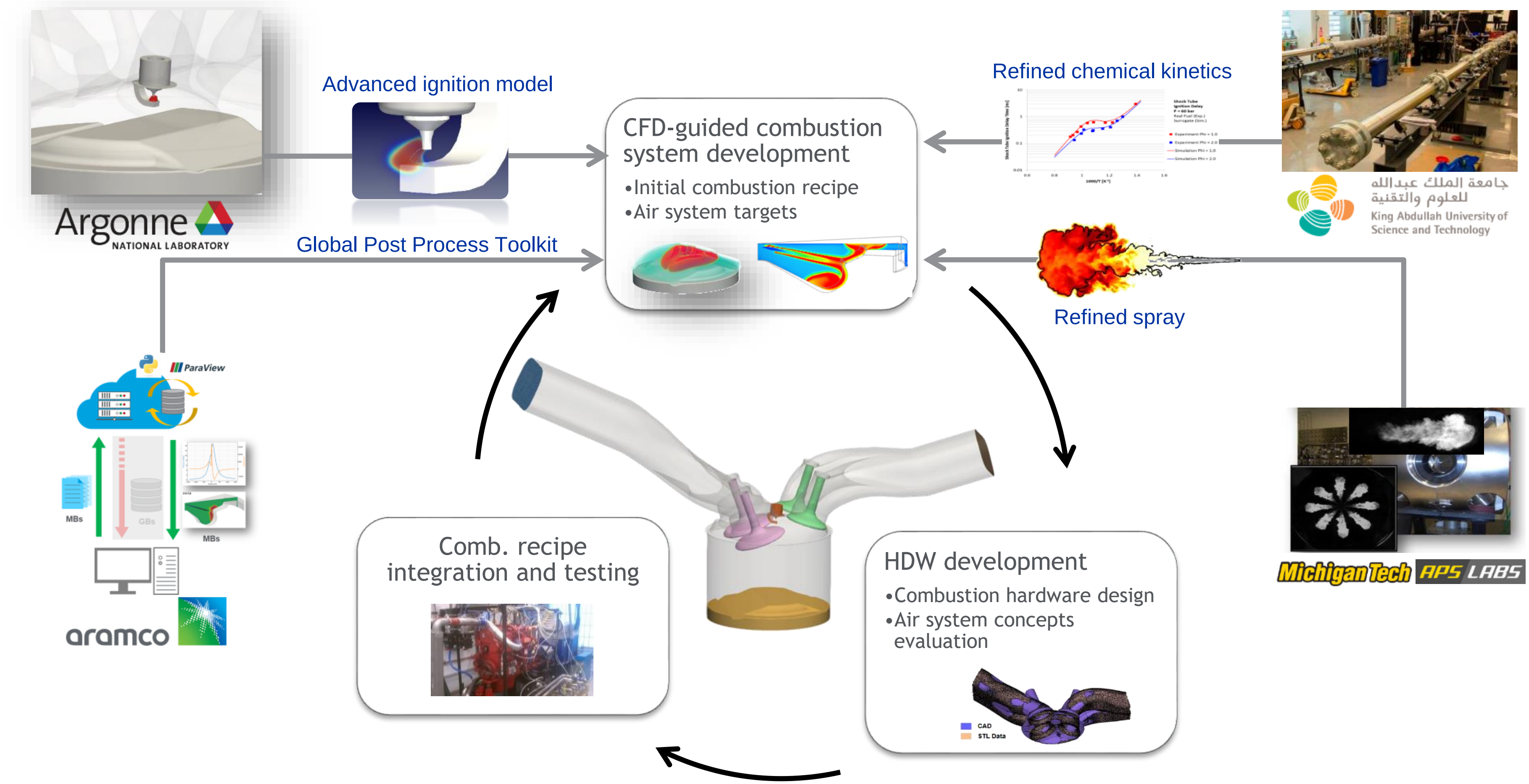
- Experimental Approach to Gasoline Range Fuels
  - *Enter gasoline physical property range while maintaining similar reactivity*
  - *Push towards market gasoline as near-term fuel solution*
  - *Identify possible GCI fuel specifications for future application*



		Test Fuels				
		ULSD	RON60 Gasoline	RON70 Gasoline	RON80 Gasoline	RON91 Gasoline
IBP	˚C	158	41	40	37	34
T10	˚C	209	71	62	57	51
T50	˚C	254	98	91	88	83
T90	˚C	**305**	**124**	**127**	**133**	**151**
FBP	˚C	336	141	169	184	198
Density at 15.56 ˚C	g/mL	**0.853**	**0.714**	**0.717**	**0.724**	**0.733**
Kinematic viscosity	cSt	**2.42**	**0.59**	**0.57**	**0.56**	**0.55**
Aromatics	vol%	29.0	9.1	13.7	19.7	25.7
Olefins	vol%	1.5	0.4	3.0	5.6	10.4
Saturates	vol%	69.5	90.5	83.4	74.7	63.9
Sulfur	ppm	5.9	19.3	8.2	6.2	3.0
H/C ratio	-	1.822	2.124	2.058	1.981	1.854
Cetane Number (CN)		**41.2**	**34.1**	**29.8**	**25.9**	**20.4**
RON	-	-	56.0	69.4	80.0	91.4
MON	-	-	55.1	67	74.9	84.6
AKI	-	-	55.6	68.2	77.4	88.0
Lower heating value	MJ/kg	42.76	44.112	43.623	43.58	43.42

➔ **Gasoline range fuels possess very similar physical properties, but different reactivity**

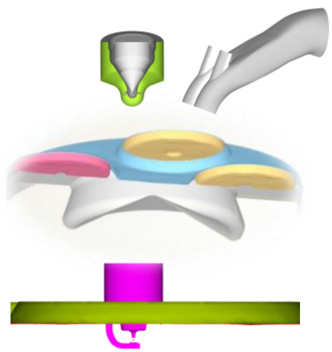
State-of-the-Art Analysis-Led Design Process



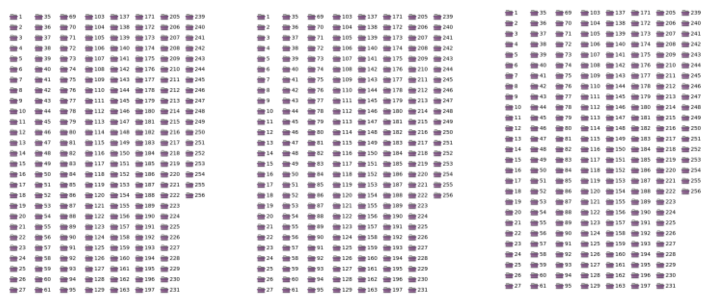
→ **Analysis-led design process is utilized for co-optimization of fuels and engines to enable robust full load range operation**

Design Optimization Methodology

Design space
- ❖Bowl geometry and CR
- ❖Injector Specs:
  - ❖Number of nozzle holes
  - ❖Injector flow rate
  - ❖Nozzle inclusion angle
- ❖Start of injection
- ❖Swirl ratio
- ❖etc.

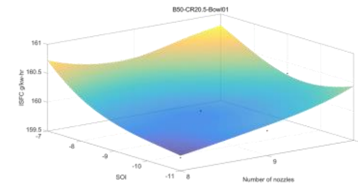


Sampling



CFD design cases at different operating conditions, 1 rack includes 16384 processors, 48 racks 786,432 processors on the 10-petaflops IBM Blue Gene/Q Mira

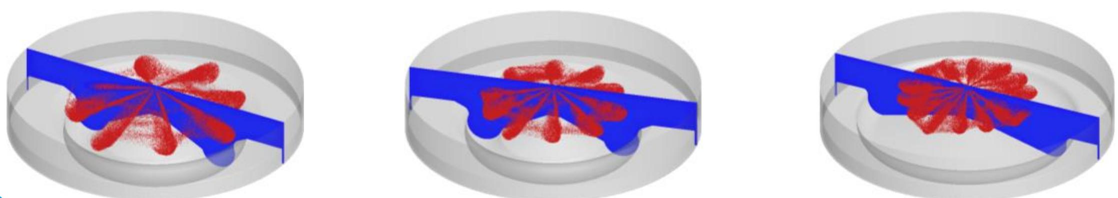
Optimization



Response Surface

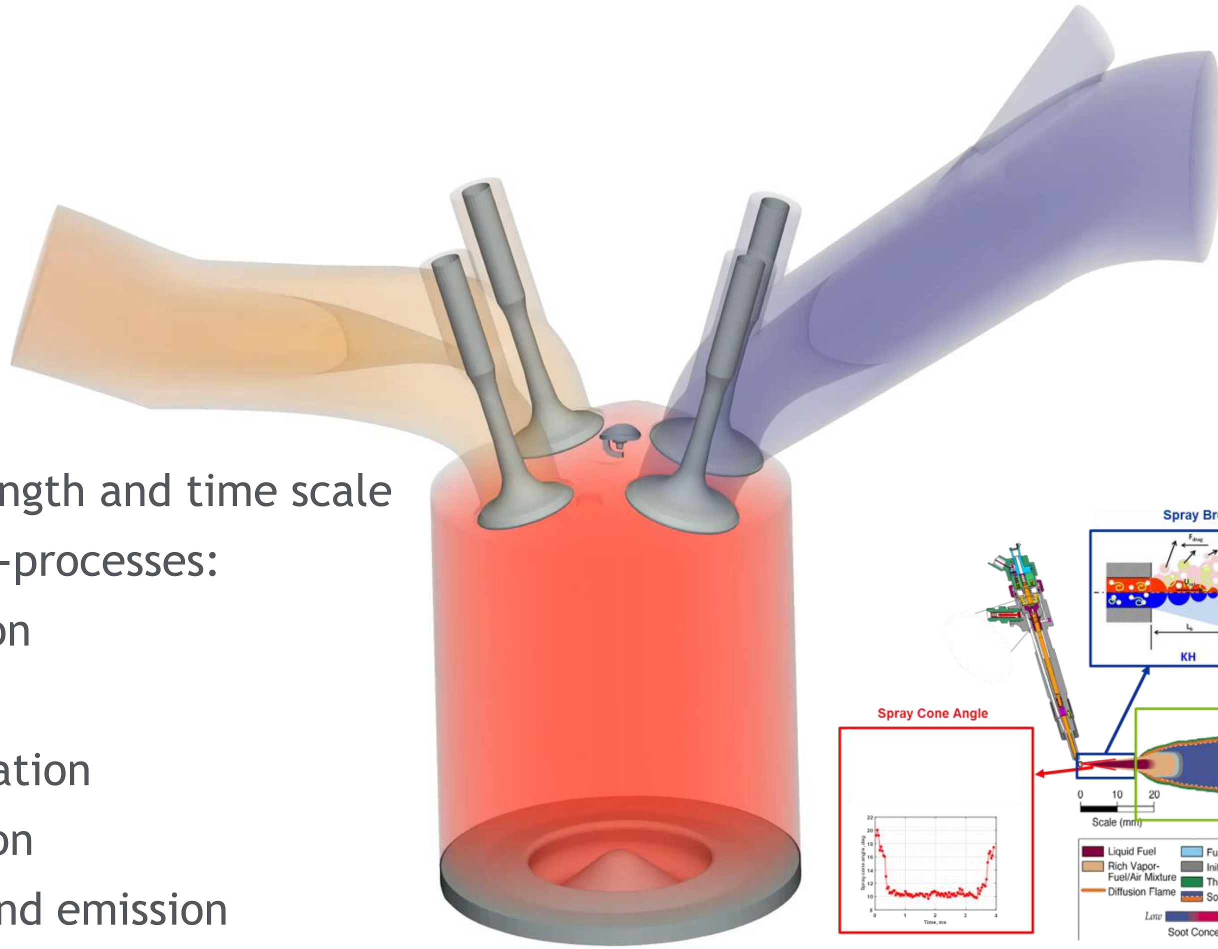
Machine Learning

Design Candidates

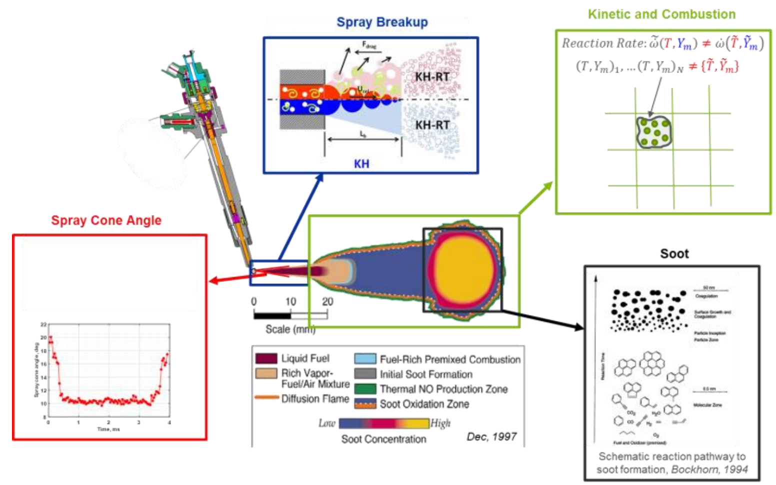


➔ Accelerated design optimization using HPC and ML

Challenges of Engine Simulations



- Disparate length and time scale
- Physical sub-processes:
  - Injection
  - Spray
  - Evaporation
- Fuel variation
- Chemistry and emission
- Load balancing

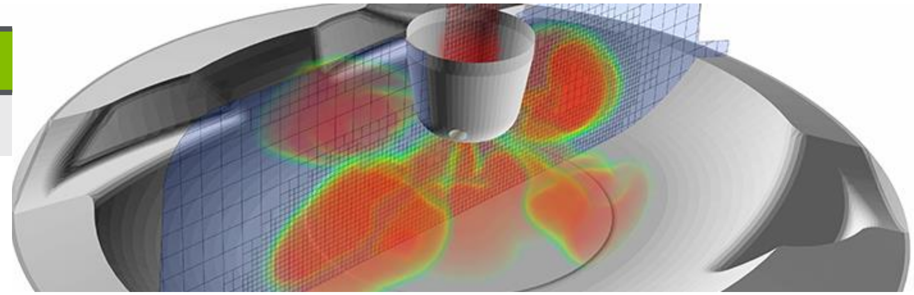


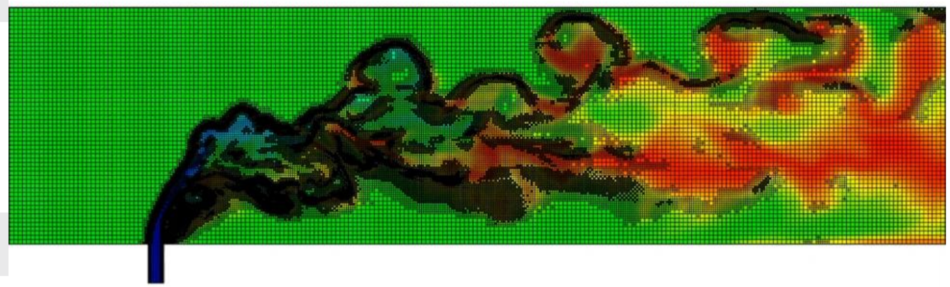
➔ Accurately simulating combustion engines is challenging, especially on supercomputer

General Use

Simulation Code - CONVERGE

CONVERGE	
Dimensionality	3D with Adaptive Mesh Refinement
Grid Details	Base grid: 1 mm Smallest grid size: 0.25 mm Gradient-based AMR on velocity and temperature Fixed embedding near nozzle region: 0.25 mm
Total Cell Count	Sector: 300,000 Full: 2.8 million
Turbulence	RNG k-ε RANS
Wall Heat Transfer	O'Rourke & Amsden
Spray Models	Injection: Blob Break-up: KH-RT Collision: No Time Counter (NTC) Evaporation: Frossling correlation Liquid properties generated from HYSYS
Time Step	Variable time step
Combustion Model	Detailed chemistry combustion model
Chemical Mechanism	Naphtha (PRF58): Liu et al. PRF mech ULSD: Chalmers n-heptane mech
Emission Models	Soot: Hiroyasu-NSC NOx: Detailed

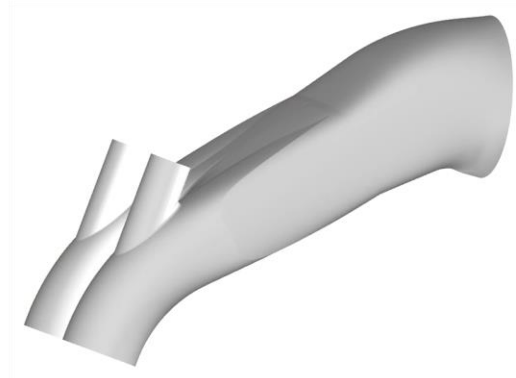


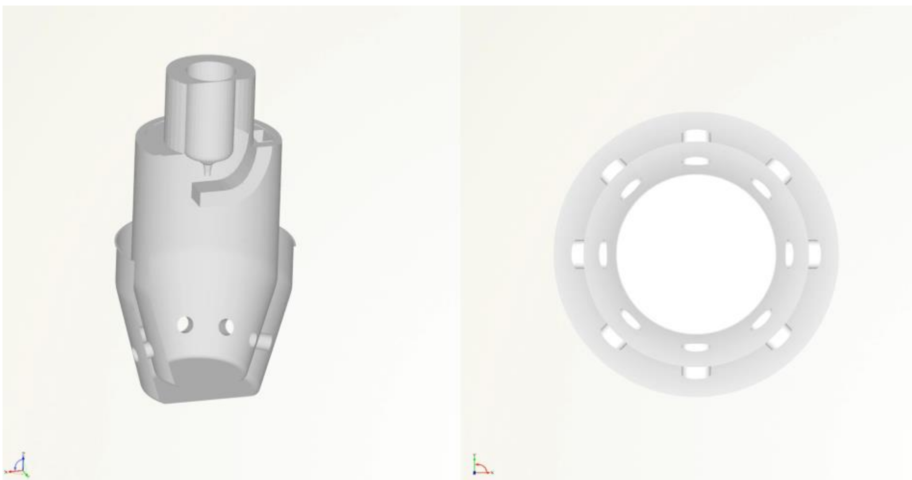


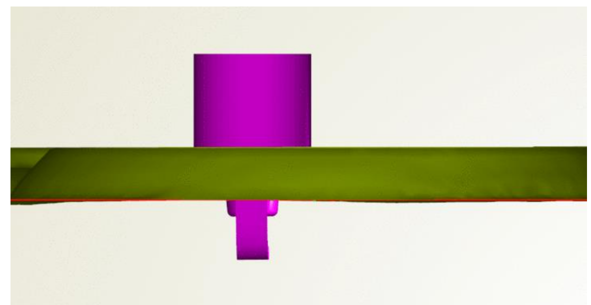
Courtesy of Convergent Science

➔ **Well-connected to automotive industry by using CONVERGE**

Automatic Geometry Generation Using CAESES

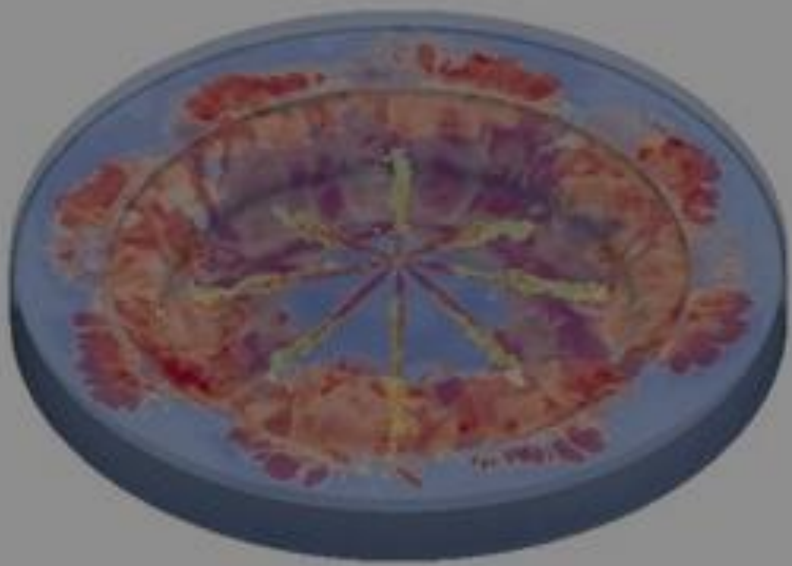






A highly specialized CAD system, CAESES, used for automatic geometry generation

General Use



Engine Combustion System Optimization[1]

- Mixing Controlled Combustion (MCC) Mode[2]

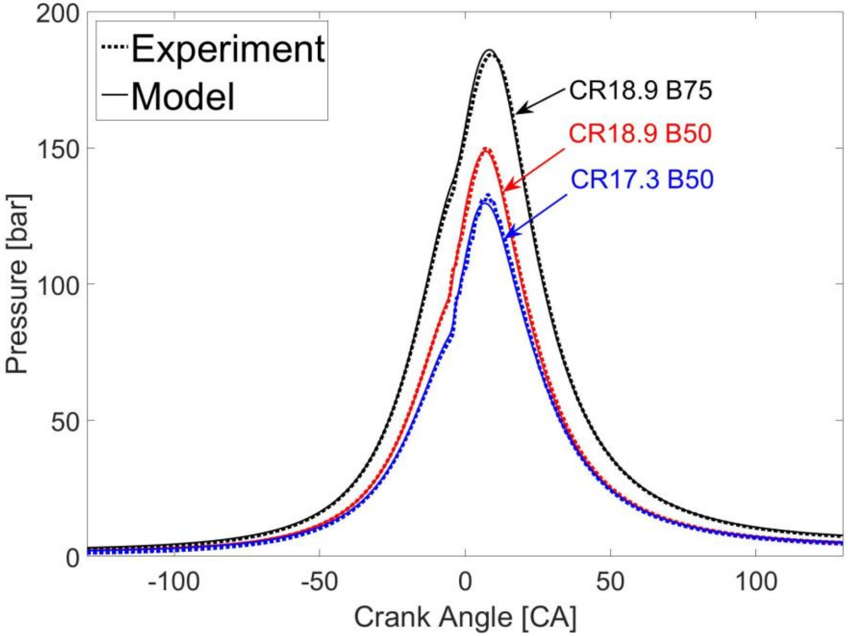
  (Near-Term – 4g/kWh NOx)

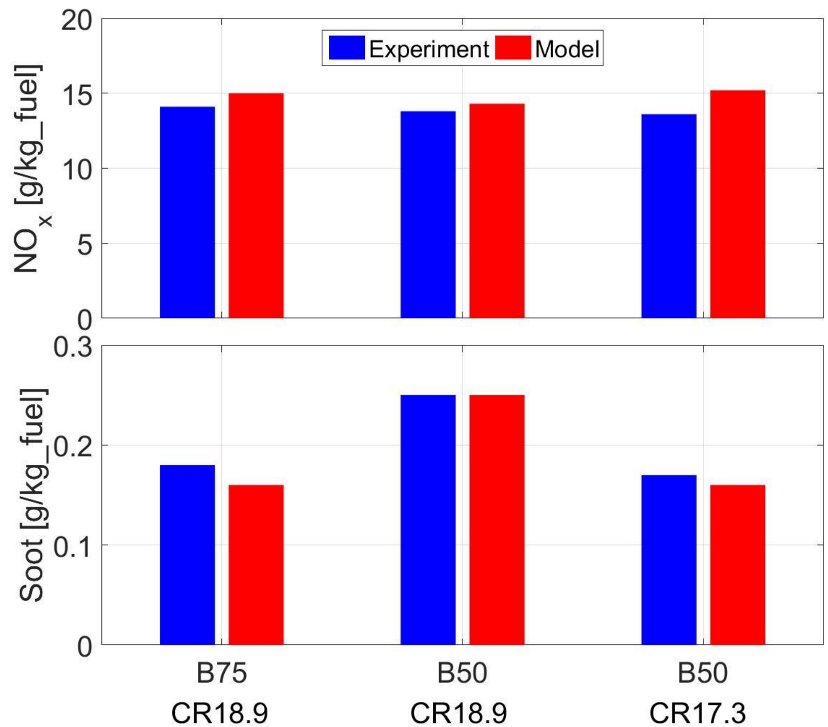
- Low Temperature Combustion (LTC) Mode[3,4]

  (Mid-Term – 1~1.5g/kWh NOx)

[1] Som, S., Pei, Y., Computing in Science & Engineering, 20(5), 77-80, 2018.
[2] Pei, Y., Zhang, Y., Kumar, P., Traver, M., Cleary, D.J. et al., *SAE Int. J. Commer. Veh.* 10(2):2017, doi:10.4271/2017-01-0550.
[3] Zhang, Y., Kumar, P., Pei, Y., Traver, M., Cleary, D., SAE Int. J. Fuels Lubs., 2018.
[4] Pei, Y., Zhang, Y., Traver, M., Cleary, D.J., Pal, P., Som, S., Futterer, C., Brenner, M., Probst, D., SAE Fuels Lubs Meeting 2019, San Antonio, USA.

Mixing Controlled Combustion - Model Correlation



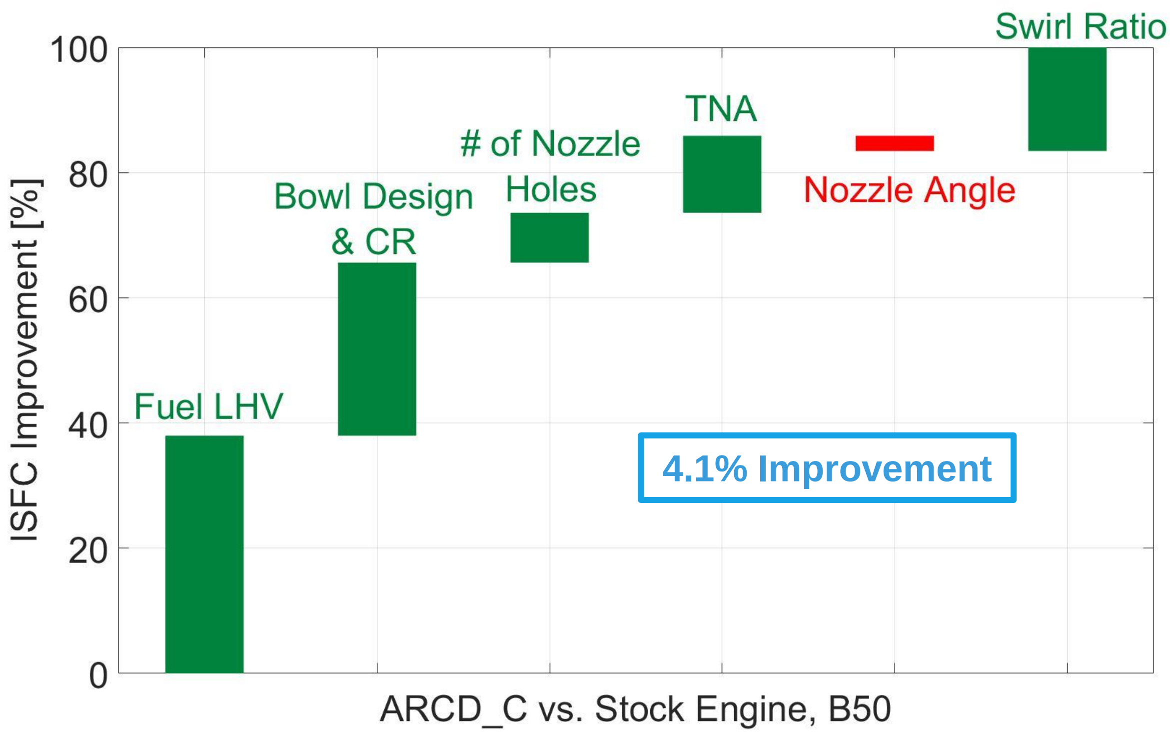


Model predictions are in reasonably good agreement with experimental data:

- Cylinder pressure trace and emissions
- Different loads and CRs

➔ **Model predictions are in reasonably good agreement with experimental data**

Mixing Controlled Combustion - Efficiency Improvement Prediction



Fuel consumption improvement at B50:

- 4.1% improvement compared to stock engine with Diesel

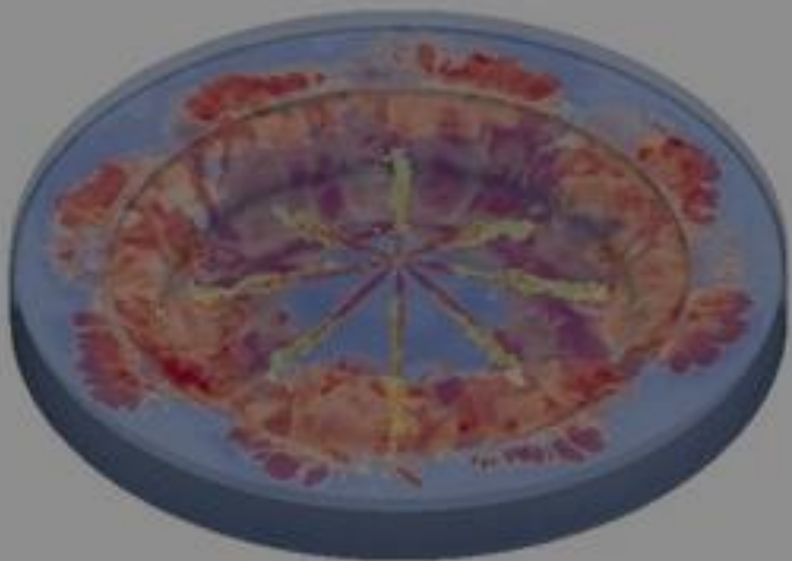
➔ **4.1% better fuel consumption calculated with optimized combustion system**

Mixing Controlled Combustion - Hardware Performance

SET 12-mode composite results	BTE [%]	BSFC [g/kWh]	BSFC improv. [%, vs. RON60 stock]	NOx [g/kWh]	Soot [g/kWh]
18.9CR_Stock	42.5	198.6	-	4.7	***0.1***
RON60_BowlC_8H_TNA1.5_SR2.0	42.5	192.3	***3.2***	4.5	***0.046***
RON60_BowlC_8H_TNA1.0_SR1.0	42.5	192.1	***3.3***	4.5	***0.029***
RON60_BowlE_9H_TNA1.3_SR1.0	42.8	190.2	***4.2***	4.5	***0.084***

- 3.2-4.2% 12-mode combined BSFC improvement
- CFD model captured the efficiency trend, but still needs improvement on soot prediction
  - Plume-to-plume interaction
  - Soot formation vs. soot oxidation

➔ High-fidelity CFD accurately guided engine design in a much more cost effective manner



Engine Combustion System Optimization[1]

- Mixing Controlled Combustion (MCC) Mode[2]

  (Near-Term – 4g/kWh NOx)

- Low Temperature Combustion (LTC) Mode[3,4]

  (Mid-Term – 1~1.5g/kWh NOx)

[1] Som, S., Pei, Y., Computing in Science & Engineering, 20(5), 77-80, 2018.
[2] Pei, Y., Zhang, Y., Kumar, P., Traver, M., Cleary, D.J. et al., *SAE Int. J. Commer. Veh.* 10(2):2017, doi:10.4271/2017-01-0550.
[3] Zhang, Y., Kumar, P., Pei, Y., Traver, M., Cleary, D., SAE Int. J. Fuels Lubs., 2018.
[4] Pei, Y., Zhang, Y., Traver, M., Cleary, D.J., Pal, P., Som, S., Futterer, C., Brenner, M., Probst, D., SAE Fuels Lubs Meeting 2019, San Antonio, USA.

Argonne NATIONAL LABORATORY

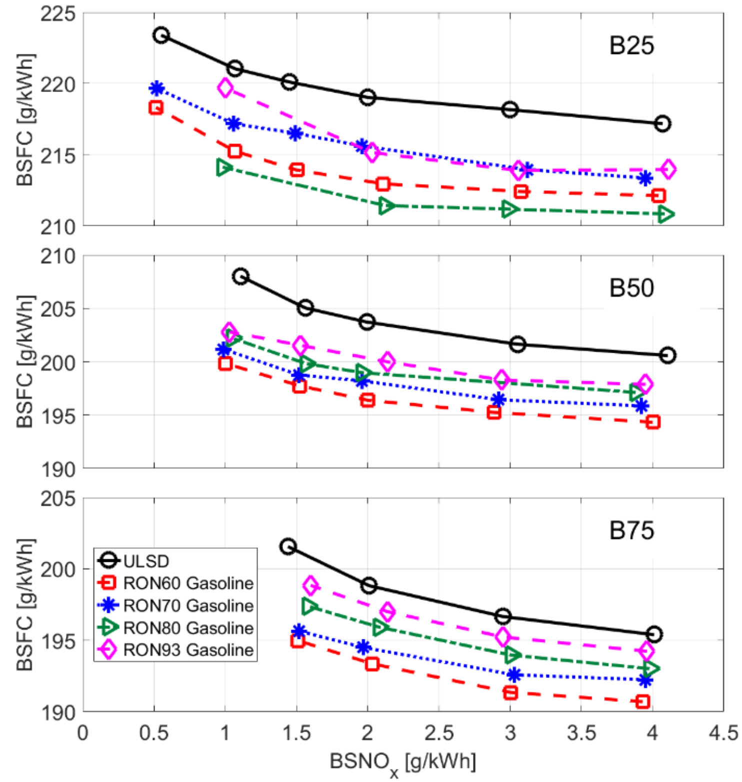
CONVERGENT SCIENCE

CAESES

Low Temperature Combustion - Engine Testing and Pre-DoE

- Extensive testing at CR 15.7 and pre-DoE conducted:
  - Leaner operation & improved air utilization
  - Improved air system will be critical

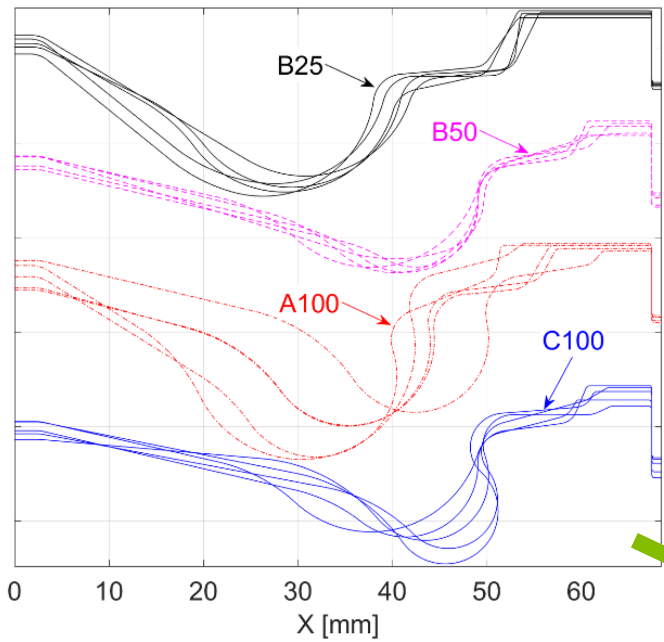
Key Design Elements	
Initial Fuel	RON80 Gasoline
CR	15.7 → 16.5
Piston Bowl Geometry	Narrower Step Bowl than Stock
Total Nozzle Area	Remain Constant
# of Nozzle Holes	Increased to 9
Spray Angle	Increased to 152
Thermal Boundary Conditions	Pivc: increased Tivc: decreased EGR: increased



BSFC for ULSD and the gasolines at CR15.7

➔ **Extensive pre-DoE conducted for 1-1.5 g/kw-hr NOx design optimization**

Low Temperature Combustion - Merit and Weight Functions



Evaluation at different conditions

	Weight (A)	Scaled Weight
B25	10	0.278
B50	10	0.278
A100	8	0.222
C100	8	0.222

EPA SET weighting (A) factors

$$Merit = 100 * \left[\frac{ISFC\_op}{ISFC} - 100 * f(PMAX) - f(MPRR) - 0.1 * f(SOOT) - f(NO_x) \right]$$

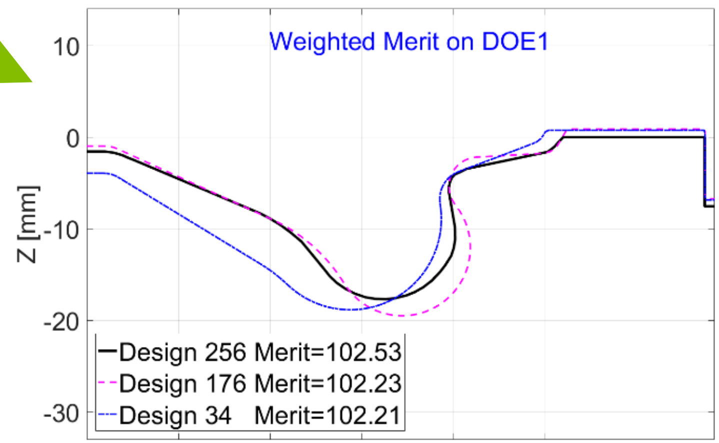
Where

$$f(PMAX) = \begin{cases} \frac{PMAX}{220} - 1, if\ PMAX > 220 \\ 0, if\ PMAX \leq 220 \end{cases}$$

$$f(MPRR) = \begin{cases} \frac{MPRR}{12} - 1, if\ MPRR > 12 \\ 0, if\ MPRR \leq 12 \end{cases}$$

$$f(SOOT) = \begin{cases} \frac{SOOT}{SOOT\_op} - 1, if\ SOOT > SOOT\_op \\ 0, if\ SOOT \leq SOOT\_op \end{cases}$$

$$f(NO_x) = \begin{cases} \frac{NO_x}{NOx\_op} - 1, if\ NO_x > NOx\_op \\ 0, if\ NO_x \leq NOx\_op \end{cases}$$



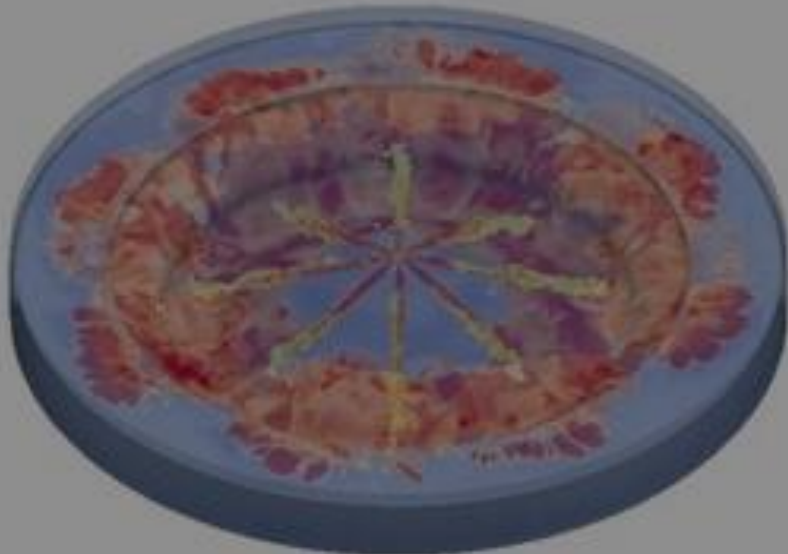
→ Merit and weight functions to harmonize the best designs at different operating conditions

Low Temperature Combustion - Efficiency Improvement Potential

	Designs	ISFC		Soot	NOx	MPRR	PCP
		[g/kWh]	[%]	[g/kWh]	[g/kWh]	[bar/CA]	[bar]
B25	baseline	172.5	-	0.046	0.80	7.4	82.0
	256	163.7	5.1	0.026	0.95	7.9	95.9
	176	165.3	4.2	0.038	0.70	8.6	94.8
	34	163.0	5.5	0.029	0.92	8.7	96.1
B50	baseline	170.7	-	0.118	0.84	10.2	122.0
	256	160.0	6.3	0.086	1.03	10.4	152.3
	176	162.2	5.0	0.116	0.88	10.3	150.6
	34	161.7	5.2	0.123	0.79	10.2	149.1
A100	256	166.0	-	0.059	1.46	10.1	216.8
	176	166.9	-	0.055	1.11	9.9	212.3
	34	166.6	-	0.060	0.97	9.7	210.5
C100	256	161.1	-	0.091	1.46	10.0	208.2
	176	162.9	-	0.103	1.19	9.9	206.0
	34	163.1	-	0.122	1.03	9.8	204.8

→ **Up to 6.3% better fuel consumption calculated with optimized combustion system**

Engine Design



Machine Learning

Machine Learning for Engine Design Optimization

[1]Moiz, A. A., Pal, P., Probst, D., Pei, Y., Zhang, Y., Som, S., and Kodavasal, J., 2018, *SAE International Journal of Commercial Vehicles*, 11(5), pp. 291-306.
[2]Probst, M.P., Raju, M., Senecal, P.K., Kodavasal, J., Pal. P., Som, S., Moiz, A.A., Pei, Y., 2019, *J. Engineer. Gas Turb. Power, 141(9).*
[3]Owoyele, O.O., Pal. P., 2019, *ASME 2019 Internal Combustion Engine Division Fall Technical Conference, Chicago, IL, USA, 2019.*
[4]Badra, J., Khaled, F., Tang, M., Pei, Y. Kodavasal, J., Pal. P., Owoyele, O., Futterer, C., Brenner, M., Farooq, A., 2019, *ASME 2019 Internal Combustion Engine Division Fall Technical Conference, Chicago, IL, USA, 2019.*

CONVERGENT SCIENCE

Argonne NATIONAL LABORATORY

Machine Learning – Genetic Algorithm (ML-GA)*

Challenge: Traditional CFD based optimization can be time-consuming
Goal: Reduce the time to design by using ML

ML model → best fit the complicated surface
GA model → find optimum over the surface

Notation	Input Parameter	min	max	units
nNoz	Number of Nozzle holes	8	10	-
TNA	Total Nozzle Area	1	1.3	-
Pinj	Injection Pressure	1400	1800	bar
SOI	Start of injection timing	-11	-7	dATDC
Nang	Nozzle Inclusion Angle	72.7	82.7	deg
EGR	EGR fraction	0.35	0.5	-
Tivc	IVC temperature	323	373	K
Pivc	IVC pressure	2.0	2.3	bar
SR	Swirl Ratio	-2.4	-1	-

CFD-GA

Run time on a cluster

12 hrs/sim →
800 sims w/ 8 per batch→
2 months

ML-GA is faster and scalable

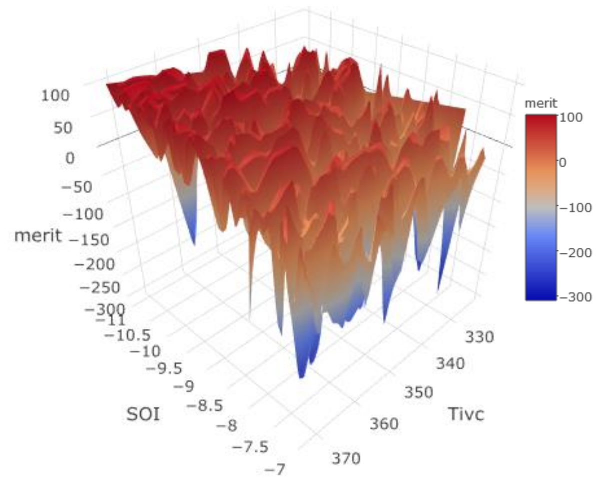
ML-GA

Run time on a SuperComputer

250 sims in one batch→
A day

Run time on a cluster

12 hrs/sim →
250 sims w/ 8 per batch→
2 weeks

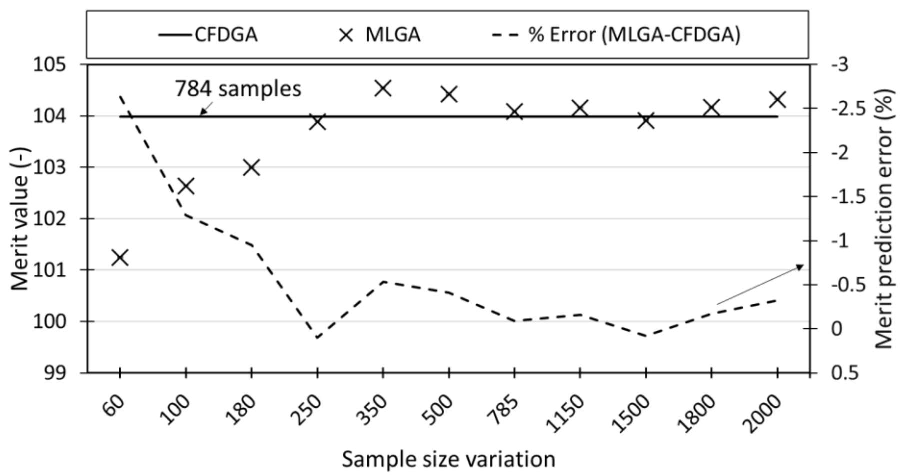


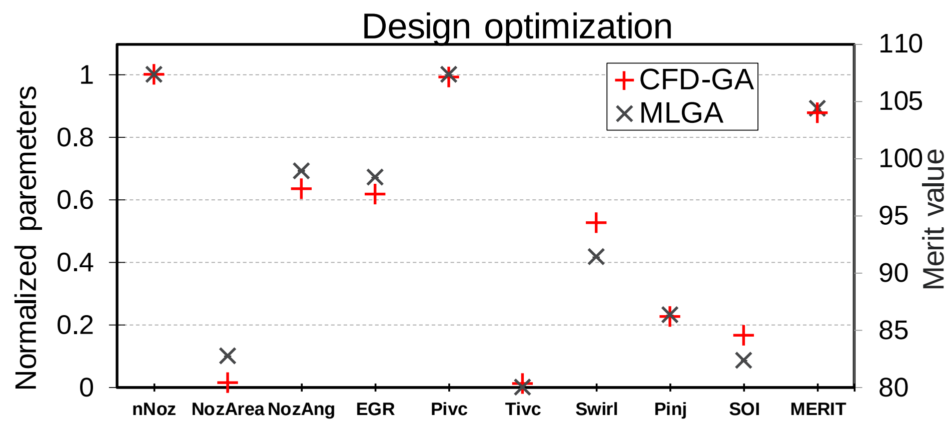
*Moiz, A. A., Pal, P., Probst, D., Pei, Y., Zhang, Y., Som, S., and Kodavasal, J., 2018, *SAE Int. J. Commer. Veh.*, 11(5), pp. 291-306.

➔ **ML-GA reduce the time to design utilizing supercomputer**

Incorporating ML Workflow into Engine Designs

- ML training data from the previous Gasoline Compression Ignition design work
- For 9 design variables, ~250 simulations sufficient to train ML
- **ML challenges are training data and uncertainty quantification and error estimation to know when our ML is a good model**





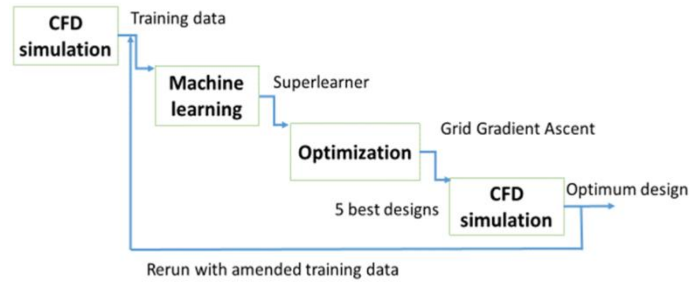
➔ ML-GA provides an alternative way of doing design optimization

General Use

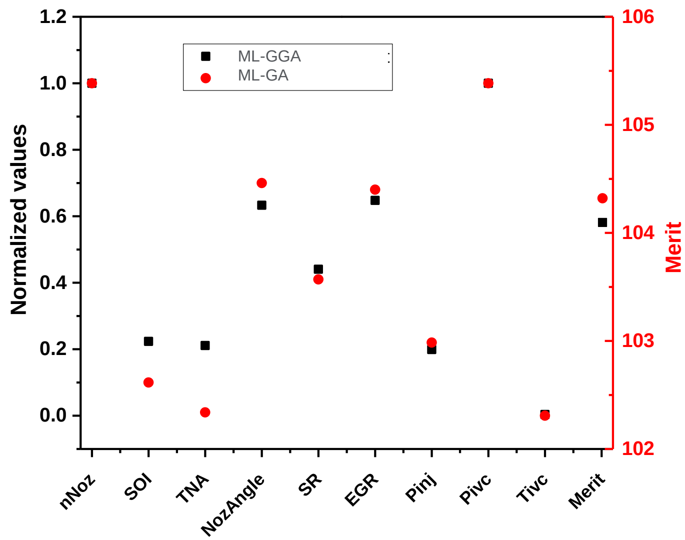
aramco

Extend to Geometry Machine Learning Optimization

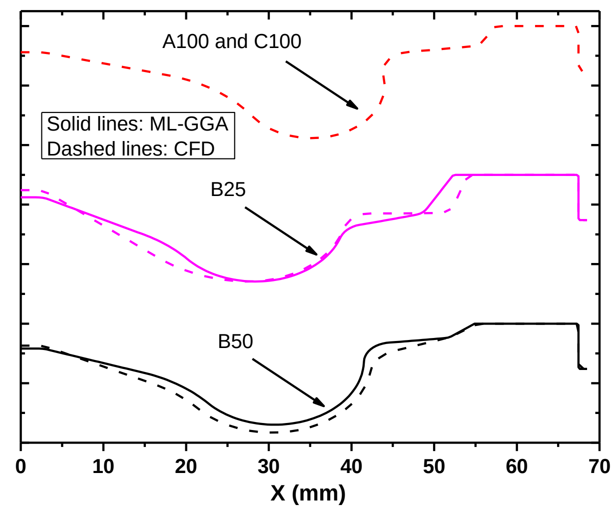
- Based upon the ML-GA approach, ML-GGA (Grid Gradient Accent) is proposed to deal with piston bowl optimization



ML-GGA piston bowl geometry optimization scheme



Optimum design by using ML-GA versus ML-GGA method



The best designs from CFD and ML-GGA for all operating points

*Badra, J., Khaled, F., Tang, M., Pei, Y. Kodavasal, J., Pal. P., Owoyele, O., Futterer, C., Brenner, M., Farooq, A., 2019, *ASME 2019 Internal Combustion Engine Division Fall Technical Conference, Chicago, IL, USA.*

➔ **ML-GA reduce the time to design utilizing supercomputer**

Summary and Future Work

- Comprehensive design optimizations were performed for a modern heavy-duty diesel engine that show significant fuel consumption improvement
- Demonstrated an accelerated CFD-guided engine design optimization using a world-leading supercomputer
- CAESES proves to be powerful in assisting engine design
- Machine learning proves to be an enabler for further reduce the time to design

Future work:

- Streamline the HPC-based design optimization process, e.g., SWIFT
- Integrate ML into the production design process

“Developing Virtual Engines” Symposium

at ASME Internal Combustion Engines Fall Meeting
13:30 – 17:45 on 10/22/2019 at Chicago, IL
Theme: Future Transportation Perspective and its Implications to Virtual Engine Development
Experts from DOE and Automotive Industries

Acknowledgement

Contributors:

- Yu Zhang, Jihad Badra, Meng Tang, Praveen Kumar, Michael Traver at Aramco
- Pinaki Pal, Ope Owoyele, Sibendu Som at Argonne National Laboratory
- Carsten Futterer, Mattia Brenner at Friendship Systems
- Daniel Probst, Kelly Senecal, Eric Pomraning, Keith Richard at Convergent Science
- Advanced Engineering System Integration team at Cummins Technical Center

Computing resources:

- MIRA at Argonne Leadership Computing Facility - Argonne National Laboratory
- ITD – Aramco Services Company for the support of computing cluster

thank you

Question & Answers

where energy is opportunity™